

# Resonance structures in the multichannel quantum defect theory for the photofragmentation processes involving one closed and many open channels

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The transformation introduced by Giusti-Suzor and Fano and extended by Lecomte and Ueda for the study of resonance structures in the multichannel quantum defect theory (MQDT) is used to reformulate MQDT into the forms having one-to-one correspondence with those in Fano's configuration mixing (CM) theory of resonance for the photofragmentation processes involving one closed and many open channels. The reformulation thus allows MQDT to have the full power of the CM theory, still keeping its own strengths such as the fundamental description of resonance phenomena without an assumption of the presence of a discrete state as in CM.

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## I. INTRODUCTION

Though multichannel quantum defect theory (MQDT) is a powerful theory of resonance capable of describing complex spectra including both bound and continuum regions with only a few parameters, resonance structures are not transparently identified in its formulation because of the indirect treatment of resonance[1, 2]. In order to identify resonance terms, one needs a special treatment like the one Giusti-Suzor and Fano introduced for the two channel case[3]. They noticed that the usual L<sub>u</sub>-Fano plot often obscures symmetry apparent in its extended version. The symmetry can be brought out in the MQDT formulation by shifting the origin of the plot to the center of symmetry using the phase-shifted base pairs first considered in Ref. [4]:

$$(f, g) \rightarrow (f \cos \pi\mu - g \sin \pi\mu, g \cos \pi\mu + f \sin \pi\mu). \quad (1)$$

By this phase renormalization, the diagonal elements of short-range reactance matrices  $K$  can be made zero so that resonance structures are separated from the background ones in two channel processes (Dubau and Seaton also obtained the same results as Giusti-Suzor and Fano's ones from a different approach[5]).

Generalizations of their method to the case involving more than two channels have been done by Cooke and Cromer[6], Lecomte[7], Ueda[8], Giusti-Suzor and Lefebvre-Brion[9], Wintgen and Fridrich[10], and Cohen[11]. Lecomte and Ueda showed that, for such a general case, making the diagonal elements of reactance matrices zero can only be achieved with an additional orthogonal transformation of basis functions besides the phase renormalization[12]. Using this transformation, Lecomte derived the best parameters for the

description of total autoionization cross-sections shorn of the background part for the most general case involving many open and many closed channels. Ueda derived total cross-section formulas analogous to Fano's resonance formula for several cases including one closed and many open channels. Giusti-Suzor and Lefebvre-Brion[9], and Wintgen and Friedrich[10] did the detailed studies for the case of two closed and one open channels and Cohen[11] involving two closed and two open channels.

One drawback of the above-mentioned work is that partial cross-section formulas for photofragmentation processes were not dealt with. Recently, Lee[13] and Lee and Kim[14] derived the MQDT formulation which yielded the partial cross-section formulas analogous to Fano's resonance formula and obtained the complete relation between MQDT and the configuration mixing (CM) formulas[15, 16, 17, 18, 19, 20, 21]. But their work was restricted to the case involving only two open and one closed channels. This paper extends their work to the case involving many open channels and has succeeded in obtaining the same degree of results as the previous ones.

Section 2 describes the reformulation. Section 3 derives the photofragmentation cross-sections. Finally, Section 4 gives the summary and discussion.

## II. REFORMULATION

In the multichannel quantum defect theory of photofragmentation process, the coordinate  $R$  for a relative motion of colliding partners along which fragmentation takes place is divided into two ranges  $R \leq R_0$  and  $R > R_0$ , the inner and outer ones, respectively. In contrast to the inner range where transfers in energy, momentum, angular momentum, spin, or the formation of a transient complex occur due to the strong interactions there, channels are decoupled in the outer range, and the motion is governed by ordinary second-order differential equations and described by superpo-

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sitions of the energy-normalized regular and irregular base pair  $(f_j(R), g_j(R))$ , or incoming and outgoing base pair  $(\exp(-ik_j R), \exp(ik_j R))$ . For an  $N$ -channel system,  $N$  independent degenerate solutions of the Schrödinger equation for the decoupled motion in  $R > R_0$  may be expressed into a standing-wave type

$$\Psi_i(R, \omega) = \sum_{j=1}^N \Phi_j(\omega) [f_j(R) \delta_{ji} - g_j(R) K_{ji}], \quad (2)$$

or an incoming-wave type

$$\Psi_i^{(-)}(R, \omega) = \sum_{j=1}^N \Phi_j(\omega) [\phi_j^+(R) \delta_{ji} - \phi_j^-(R) S_{ji}], \quad (3)$$

where  $\Phi_j(\omega)$  are the channel basis functions for the coordinate space excluding  $R$  and  $\phi_j^\pm$  defined as  $(\pm f_j + i g_j)/2$ .  $K_{ji}$  and  $S_{ji}$  denote the  $(j, i)$ -elements of short-range reactance and scattering matrices, respectively, and are related with each other in matrix notation by  $S = (1 - iK)(1 + iK)^{-1}$  ( $S$  is here taken as a complex conjugate of the usual definition, for convenience). Using the quantum defect theory parameters  $\eta_j$ ,  $\beta_j$ , and  $D_j$  in Ref. [22] for an arbitrary field,  $\phi_j^\pm$  are given in the outer range  $R > R_0$  by  $-i(m_j/2\pi k_j)^{1/2} \exp(\pm i\eta_j) f_j^\pm$  for open channels and  $\mp(m_j/\pi\kappa_j)^{1/2} \exp(\pm i\beta_j)(D_j f_j^\pm \pm iD_j^{-1} f_j^\mp)/2$  for closed channels, where  $f_j^\pm$  denote  $\exp(\pm ik_j R)$ .

Though all the  $N$  solutions are needed to describe the motion in the intermediate range, some of them become closed and no longer exist in the limit of  $R \rightarrow \infty$ . In the present work, we will consider the case involving only one closed and many, say  $N_0$ , open channels at large  $R$ , i.e.  $N = N_0 + 1$ . We will denote the set of open channels by  $P$  and that of closed ones by  $Q$ . Open channels will be marked with  $1, 2, \dots, N_0$  and the following single closed channel with  $c$  instead of  $N$  for easy recognition. Though meaningful only at large  $R$ , still it may be convenient to keep the classification of channels as open or closed in the intermediate range. The wavefunction for the photofragmentation process into the  $i$ -th fragmentation channel, denoted as  $\Psi_i^{(-)}$ , should satisfy the incoming-wave boundary condition  $\Psi_i^{(-)} \rightarrow \sum_{j \in P} \Phi_j(\phi_j^+ \delta_{ji} - \phi_j^- S_{ji})$  at large  $R$  [23] and can be obtained by making a linear combination of incoming channel basis functions  $\Psi_i^{(-)}$  of Eq. (3), substituting the explicit forms for  $\phi_j^\pm$  given above and then setting the coefficients of exponentially rising terms to zero. This procedure yields  $\mathbf{S} = S^{oo} - S^{oc}(S^{cc} - e^{2i\beta})^{-1}S^{co}$ , where the indices  $o$  and  $c$  stand for open and closed components, respectively. The second term shows that resonances come from the pole structure of the inverse matrix  $[S^{cc} - \exp(2i\beta)]^{-1}$  due to the closed channel. The first term  $S^{oo}$ , which contain couplings only among open channels, cannot be regarded as corresponding to the background one in the usual resonance theory such as the configuration mixing method (CM) of Fano[15] because

of its failure to satisfy the unitary condition. To find the corresponding one to the background scattering matrix  $\mathbf{S}_B$  of CM, we rewrite the physical scattering matrix  $\mathbf{S}$  into a form more analogous to that of CM as

$$\mathbf{S} = \sigma^{oo} + 2i \frac{(1 + iK^{oo})^{-1} K^{oc} K^{co} (1 + iK^{oo})^{-1}}{\tan \beta + \kappa^{cc}}, \quad (4)$$

where  $\kappa^{cc}$  is a new kind of complex reactance matrix studied extensively by Lecomte and defined by  $S^{cc} = (1 - i\kappa^{cc})(1 + i\kappa^{cc})^{-1}$  [7]. The new scattering matrix  $\sigma^{oo}$  in Eq. (4) is defined as  $K^{oo} = -i(1 + \sigma^{oo})^{-1}(1 - \sigma^{oo})$  and, now pleasingly, unitary. From the definition, both symmetric  $\sigma^{oo}$  and  $K^{oo}$  are simultaneously diagonalized as  $U \exp(-2i\delta^0) U^T$  and  $U \tan \delta^0 U^T$ , respectively, by the same orthogonal matrix  $U$ . Eq. (4) then becomes

$$\mathbf{S} = U e^{-i\delta^0} \left( 1 + 2i \frac{\boldsymbol{\xi} \boldsymbol{\xi}^T}{\tan \beta + \kappa^{cc}} \right) e^{-i\delta^0} U^T, \quad (5)$$

where  $\boldsymbol{\xi}$  denotes the column vector given by  $\cos \delta^0 U^T K^{oc}$ . Notice that  $\boldsymbol{\xi}^T \boldsymbol{\xi} = K^{co} (1 + K^{oo2})^{-1} K^{oc} = -\Im(\kappa^{cc})$ , which is a scalar here, but generally a matrix and plays the key role in Lecomte's work [7]. Since  $\boldsymbol{\xi}^T \boldsymbol{\xi}$  is positive definite, it can be denoted as  $\boldsymbol{\xi}^T \boldsymbol{\xi} = \xi^2$ . Elements of the column vector  $\boldsymbol{\xi}$  are real but cannot be made positive, in general, by redefining  $U$  since the latter is restricted by  $\det U = 1$ . The sum of their squares is equal to  $\xi^2$ , i.e.  $\sum_i \xi_i^2 = \xi^2$ .

In order to utilize Hazi's theorem that, for an isolated resonance in a multichannel system, sum of eigenphases satisfies the resonance behavior of an elastic phase shift, the determinant of  $\mathbf{S}$  is calculated by making use of the mathematical techniques in his paper [24] as

$$\det(\mathbf{S}) = e^{-2i\delta_\Sigma^0} \left( \frac{\tan \beta + \kappa^{cc*}}{\tan \beta + \kappa^{cc}} \right), \quad (6)$$

where  $\delta_\Sigma^0$  denotes the sum of eigenphases of  $\sigma^{oo}$ , i.e.  $\sum_j \delta_j^0$ . If we let  $\det(\mathbf{S}) = \exp(-2i\delta_\Sigma)$  with  $\delta_\Sigma = \sum_j \delta_j$ , then  $\exp[-2i(\delta_\Sigma - \delta_\Sigma^0)] = (\tan \beta + \kappa^{cc*})/(\tan \beta + \kappa^{cc})$  and one obtains

$$\tan(\delta_\Sigma - \delta_\Sigma^0) [\tan \beta + \Re(\kappa^{cc})] = \Im(\kappa^{cc}) = -\xi^2. \quad (7)$$

Following the lead of Giusti-Suzor and Fano [3], we may try to separate out geometrical factors from channel coupling strength by translating axes to make the Lu-Fano-like plot for  $\delta_\Sigma$  vs.  $\beta$  symmetrical by the phase renormalization described in Eq. (1). By the latter procedure, part of the dynamics manifested in the short-range reactance and scattering matrices  $K$  and  $S$  move into base pairs for motions in decoupled channels. The net effect is to transform the phase shifts  $\eta_j$  ( $j = 1, \dots, N_0$ ) and  $\beta$  of the original base pairs for open and closed channels into  $\eta_j' = \eta_j + \pi\mu_j$  and  $\beta' = \beta + \pi\mu_c$ , respectively. We will call the new representation, in which the Lu-Fano-like plot for  $\delta_\Sigma$  vs.  $\beta$  is symmetrical, the tilde representation.

The associated dynamical parameters will be accented by the tilde. Then

$$\tan \tilde{\delta}_\Sigma \tan \tilde{\beta} = \Im(\tilde{\kappa}^{cc}) = -\tilde{\xi}^2 \quad (8)$$

with  $\tilde{\delta}_\Sigma^0 = 0$  and  $\Re(\tilde{\kappa}^{cc}) = 0$ . Eq. (8) implies that we can identify  $\tilde{\delta}_\Sigma$  with the phase shift  $\delta_r$  due to the resonance. For isolated resonances,  $\delta_r$  varies as a function of energy as  $\cot \delta_r = -\epsilon_r \equiv -2(E - E_0)/\Gamma$ . Notice that Eq. (8) holds for all the resonances belonging to the same closed channel, yielding the extension of the definition of  $\delta_r$  from  $\cot \delta_r = -\epsilon_r$  to  $\cot \delta_r = -\tan \tilde{\beta}/\tilde{\xi}^2$ . Here, we observe that there are infinite sets of  $\{\mu_1, \dots, \mu_{N_0}\}$  satisfying  $\tilde{\delta}_\Sigma^0 = \delta_\Sigma^0 + \pi\mu_\Sigma = 0$  and thus yielding Eq. (8). A convenient choice may be  $\mu_1 = \mu_\Sigma$  and  $\mu_j = 0$  ( $j = 2, \dots, N_0$ ). Let us denote this particular set by  $\mu_\Sigma^c$ . Observables are not affected by this arbitrariness as we will see later.

Now let us consider obtaining  $\mu_\Sigma$  and  $\mu_c$  which give rise to the tilde representation. The value of  $\mu_c$  which yields  $\Re(\tilde{\kappa}^{cc}) = 0$  is easily obtained as  $\tan 2\pi\mu_c = 2\Re(\kappa^{cc})/(1 - |\kappa^{cc}|^2)$  from the transformation relation  $\tilde{\kappa}^{cc} = (\kappa^{cc} \sin \pi\mu_c + \cos \pi\mu_c)^{-1}(\kappa^{cc} \cos \pi\mu_c - \sin \pi\mu_c)$  derived by Lecomte[7]. It may be expressed more compactly in terms of  $S^{cc}$  as  $\exp(-2i\pi\mu_c) = S^{cc}/|S^{cc}|$ , indicating that the phase of  $S^{cc}$  is removed so as to make  $\tilde{S}^{cc}$  real and subsequently  $\tilde{\kappa}^{cc}$  pure imaginary. Next, let us consider obtaining  $\mu_\Sigma$  which yields  $\tilde{\delta}_\Sigma^0 = 0$ . Under the phase renormalization,  $\sigma^{oo}$  is transformed into  $\tilde{\sigma}^{oo} = \exp(i\pi\mu^o) \{S^{oo} - S^{oc}S^{co}/[S^{cc} + \exp(-2i\pi\mu_c)]\} \exp(i\pi\mu^o)$ . Then, the determinant of  $\tilde{\sigma}^{oo}$  is calculated as  $\exp(2i\pi\mu_\Sigma) [\det(S) + \exp(-2i\pi\mu_c) \det(S^{oo})]/[S^{cc} + \exp(-2i\pi\mu_c)]$ . Since  $\tilde{\delta}_\Sigma^0 = 0$ ,  $\det(\tilde{\sigma}^{oo})$  equals unity and one obtains the formula for  $\exp(2i\pi\mu_\Sigma)$  as  $[S^{cc} + \exp(-2i\pi\mu_c)]/[\exp(-2i\pi\mu_c) \det(S^{oo}) + \det(S)]$ , where  $\exp(-2i\pi\mu_c) = S^{cc}/|S^{cc}|$  as already obtained. This formula for  $\exp(2i\pi\mu_\Sigma)$  may be used to obtain the relation between  $\tilde{\xi}^2$  and  $\xi^2$  in conjunction with the relations  $\det(S) = \exp[-2i\pi(\mu_\Sigma + \mu_c)]$  and  $\det(S^{oo}) = \exp(-2i\pi\mu_\Sigma)(1 - \xi^2)/(1 + \xi^2)$  available after studying the transformation (11) later. By substituting the relations into the formula, we obtain  $\tilde{\xi}^2 = 2\xi^2/\{1 + |\kappa^{cc}|^2 + [(1 + |\kappa^{cc}|^2)^2 - 4\xi^4]^{1/2}\}$ . It can be expressed more compactly in terms of  $|S^{cc}|$  as  $\tilde{\xi}^2 = (1 - |S^{cc}|)/(1 + |S^{cc}|)$ , indicating  $\tanh \pi\alpha = \tilde{\xi}^2$  if  $S^{cc}$  is parameterized with Dubau and Seaton's complex quantum defect  $\mu_c - i\alpha$  as  $\exp[-2i\pi(\mu_c - i\alpha)]$ [5], which is equivalent to Eq. (35) of Ref. [3]. Notice that  $\tilde{\xi}^2 \leq 1$ . If  $|\Im(\tilde{\kappa}^{cc})| > 1$ , Eq. (8) could be transformed into  $\tan \tilde{\delta}'_\Sigma \tan \tilde{\beta}' = 1/\Im(\tilde{\kappa}^{cc})$  with  $\tilde{\delta}_\Sigma = \tilde{\delta}'_\Sigma + \pi/2$  and  $\tilde{\beta} = \tilde{\beta}' + \pi/2$  as described in Ref. [3]. In this case,  $\tilde{\xi}^2$  might be identified with  $-1/\Im(\tilde{\kappa})$ .

In contrast to the two channel case[3], making the Lu-Fano-like plot symmetrical is not enough to separate out the strength of channel coupling from the geometrical parameters in the short-range reactance matrix, as evidenced by the nonzero  $K^{oo}$  and  $K^{cc}$ . If there are more than two open channels,  $K^{oo}$  cannot be made zero with  $\mu_\Sigma$  alone. The transformation to make both  $K^{oo}$  and

$K^{cc}$  zero was devised by Lecomte and Ueda[7, 8] by extending the transformation of Giusti-Suzor and Fano. In the present work, their prescription to make both reactance submatrices zero is a little modified in order to utilize the resonance structure in the sum of the eigenphase shifts as stated above. Let us briefly describe their transformation. It is conveniently expressed in terms of  $\phi_j^\pm$  as  $\Phi_j \phi_j'^\pm = \sum_i \Phi_i \phi_i^\pm W_{ij} \exp(\pm i\pi\mu_j)$ , where  $W$  is an orthogonal matrix with  $W^{co}$  and  $W^{oc}$  set to zero. Then,  $W^{cc}$  is just unity for the one closed channel case. This leaves orthogonal transformations only among base pairs of open channels. The second term  $\exp(\pm i\pi\mu_j)$  induces the phases to be renormalized as  $\eta_j' = \eta_j + \pi\mu_j$  ( $j = 1, \dots, N_0$ ) for open channels and as  $\beta' = \beta + \pi\mu_c$  for the closed channel. The transformation is conveniently denoted by Lecomte as  $T(\pi\mu^c, \pi\mu^o, W^{oo})$ , where  $\mu^o$  is a set of  $\mu_1, \dots, \mu_{N_0}$ . For the transformation composed of two successive operations like  $T(0, \tilde{\delta}^o, \tilde{U})T(0, 0, U_r)$  of diagram (11), consult Appendix A.

Now let us go back to the problem of finding the transformation which makes  $\tilde{K}^{oo}$  and  $\tilde{K}^{cc}$  zero. Though this problem is already solved by Lecomte[7], let us give a brief description of it for the subsequent description. With  $T(0, \pi\mu^o, W^{oo})$ ,  $\tilde{K}^{oo}$  is transformed into  $\tilde{K}'^{oo} = (\tilde{K}_W \sin \pi\mu^o + \cos \pi\mu^o)^{-1}(\tilde{K}_W \cos \pi\mu^o - \sin \pi\mu^o)$  where  $\tilde{K}_W = W^{ooT} \tilde{K}^{oo} W^{oo}$ . Let  $\tilde{U}$  diagonalize  $\tilde{K}'^{oo}$ , i.e.,  $\tilde{U}^T \tilde{K}'^{oo} \tilde{U} = \tan \tilde{\delta}^0$ . Then,  $T(0, \tilde{\delta}^0, \tilde{U})$  transforms  $\tilde{K}^{oo}$  into a zero matrix.  $\tilde{K}^{cc}$  is transformed into zero too as a by-product, which derives from two theorems. First,  $\tilde{\kappa}^{cc}$  does not change value under any transformation with  $\mu_c = 0$ . Therefore,  $\Re(\tilde{\kappa}^{cc}) = 0$  remains invariant under  $T(0, \tilde{\delta}^0, \tilde{U})$ . Secondly,  $\kappa^{cc} = K^{cc} - iK^{co}K^{oc}$  if  $K^{oo} = 0$ , whereby one has  $K^{cc} = \Re(\kappa^{cc})$ .

Let us call the new representation generated by  $T(0, \tilde{\delta}^0, \tilde{U})$  the bar-representation. In this case, the physical scattering matrix  $\tilde{S}$  becomes  $1 - 2i \exp(-i\delta_r) \sin \delta_r \tilde{\xi} \tilde{\xi}^T / \tilde{\xi}^2$ . Since  $\tilde{\xi} \tilde{\xi}^T$  is a  $N_0 \times N_0$  symmetric matrix of rank 1, it can be diagonalized by some orthogonal matrix, say  $U_r$ , as

$$U_r \tilde{\xi} \tilde{\xi}^T U_r^T = \tilde{\xi}^2 \begin{pmatrix} 1 & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 0 \end{pmatrix} \equiv \tilde{\xi}^2 \mathbf{p}_r, \quad (9)$$

where  $\mathbf{p}_r$  satisfies the property of a projection matrix. If we put  $U_r^T \mathbf{p}_r U_r = \mathbf{P}_r$ ,  $\tilde{S}$  can be written as  $\exp(-2i\delta_r \mathbf{P}_r)$ , which suggests a new representation where the physical scattering matrix is diagonal as  $\exp(-2i\delta_r \mathbf{p}_r)$ . It is easily seen that the new representation is generated by  $T(0, 0, U_r)$ . Let us call the new representation the r-representation. In this representation, the short-range  $N \times N$  reactance matrix  $K_r$  has only two nonzero elements whose value is just the strength of channel cou-

pling:

$$K_r = \begin{pmatrix} 0 & 0 & \dots & \xi \\ 0 & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ \xi & 0 & \dots & 0 \end{pmatrix}. \quad (10)$$

With this  $K_r$ , only  $\Psi_{r1}$  and  $\Psi_{rc}$  have coupling terms (recall that  $c$  is actually  $N$ ).  $\Psi_{r1}$  is dubbed the ‘effective continuum’ by others[6] and corresponds to Fano’s ‘a’ state  $\psi_E^{(a)}$ [16].  $\bar{S}$  and  $\bar{S}_r$  only contain the resonant dynamics and may be expressed as  $\exp(-2i\delta_r \bar{\kappa}^{oo}/\bar{\kappa}^{cc})$  and  $\exp(-2i\delta_r \kappa_r^{oo}/\kappa_r^{cc})$ , respectively. The process described so far can be summarized in the following diagram:

$$\begin{aligned} & \begin{cases} K \\ \delta_\Sigma^0 \neq 0 \\ \Re(\kappa^{cc}) \neq 0 \\ \Im(\kappa^{cc}) = -\xi^2 \\ \Re(\kappa^{oo}) \neq 0 \\ \beta \end{cases} \xrightarrow{T(\pi\mu_c, \pi\mu_\Sigma, I^{oo})} \begin{cases} \tilde{K} \\ \tilde{\delta}_\Sigma^0 = 0 \ (\tilde{\sigma}^{oo} = 1) \\ \Re(\tilde{\kappa}^{cc}) = 0 \\ \Im(\tilde{\kappa}^{cc}) = -\tilde{\xi}^2 \\ \Re(\tilde{\kappa}^{oo}) \neq 0 \\ \tilde{\beta} = \beta + \pi\mu_c \end{cases} \\ & \xrightarrow{T(0, \tilde{\delta}^0, \tilde{U})} \begin{cases} \tilde{K} \\ \tilde{\delta}_\Sigma^0 = 0 \ (\tilde{\sigma}^{oo} = 1) \\ \Re(\tilde{\kappa}^{cc}) = 0 \\ \Im(\tilde{\kappa}^{cc}) = -\tilde{\xi}^2 \\ \Re(\tilde{\kappa}^{oo}) = 0, \ \Im(\tilde{\kappa}^{oo}) = -\tilde{\xi}^2 \mathbf{P}_r \\ \tilde{\beta} = \tilde{\beta} \end{cases} \\ & \xrightarrow{T(0, 0, U_r)} \begin{cases} K_r \\ \delta_{r\Sigma}^0 = 0 \ (\sigma_r^{oo} = 1) \\ \Re(\kappa_r^{cc}) = 0 \\ \Im(\kappa_r^{cc}) = -\xi^2 \\ \Re(\kappa_r^{oo}) = 0, \ \Im(\kappa_r^{oo}) = -\xi^2 \mathbf{P}_r \\ \beta_r = \tilde{\beta} \end{cases}, \quad (11) \end{aligned}$$

where the set  $\mu_\Sigma^c$  is given by  $\{\mu_\Sigma, 0, \dots, 0\}$  as introduced before. Once made symmetrical by the translation of the axes, the graph of  $\delta_\Sigma$  vs.  $\tilde{\beta}$  remains moveless under further transformations  $T(0, \tilde{\delta}^0, \tilde{U})$  and  $T(0, 0, U_r)$ . We will call this kind of representations, which share the identical location of the graph on the plot, the resonance-centered representation hereinafter. The departure of our procedure from Lecomte’s one lies in that  $K^{oo}$  is not made into a zero matrix as the first step but only phases are renormalized so as to symmetrize the plot for  $\delta_\Sigma$  vs.  $\tilde{\beta}$ . This offers several advantages. The background part eliminated in the last two representations of diagram (11) is nothing but disentangled by the first process, enabling us to identify its MQDT form. The fact that the last two transformations operate only on the open channel set indicates that the resonance effect due to the closed channel is already fully accounted for by the phase renormalization alone. This enables us to separate out the background and resonant contributions in the partial cross-section formulas, which is the topic of the next section.

### III. PHOTOFRAGMENTATION CROSS-SECTION FORMULAS

Let us consider the photofragmentation processes from an initial bound state to the  $j$ -th fragment one. The

fragment state may be described by an incoming-wave as follows[7, 14]

$$\Psi_j^{(-)} = \Psi_j^{(-)} + \Psi_c^{(-)} \left[ \frac{\tan \beta + i}{\tan \beta + \kappa^{cc}} K^{co} (-i + K^{oo})^{-1} \right]_{cj}. \quad (12)$$

Notice that the term  $(\tan \beta + i)(\tan \beta + \kappa^{cc})^{-1}$  is the same for all the resonance-centered representations as  $(\tan \beta + i)[\tan \beta + i\Im(\kappa^{cc})]^{-1}$  and is very energy-sensitive as can be seen from its another expression  $-(i/\tilde{\xi})(d\delta_r/d\tilde{\beta})^{1/2} \exp[-i(\tilde{\beta} + \delta_r)]$  obtainable from it by means of  $\tan \tilde{\beta} \tan \delta_r = -\tilde{\xi}^2$ . Let us introduce new short-range wavefunctions  $M_j^{(-)}$  and  $N_j^{(-)}$  defined only for open channels by

$$\begin{aligned} M_j^{(-)} &= \Psi_j^{(-)} + \Psi_c^{(-)} [K^{co} (-i + K^{oo})^{-1}]_{cj}, \\ N_j^{(-)} &= \Psi_j^{(-)} + \frac{i}{\kappa^{cc}} \Psi_c^{(-)} [\tilde{K}^{co} (-i + \tilde{K}^{oo})^{-1}]_{cj}. \end{aligned} \quad (13)$$

Using these wavefunctions, the square of the modulus of the transition dipole moment  $\mathbf{D}_j^{(-)} \equiv (\Psi_j^{(-)} | T | i)$  may be expressed as

$$|\mathbf{D}_j^{(-)}|^2 = |(\tilde{M}_j^{(-)} | T | i)|^2 \frac{|\tan \beta + \Re(\kappa^{cc})/\xi^2 + q_j|^2}{[\tan \beta + \Re(\kappa^{cc})]^2/\xi^4 + 1}, \quad (14)$$

where  $T$  is the dipole moment operator,  $i$  stands for the initial bound state, and the complex line profile index parameter  $q_j$  is given by  $q_j = i(N_j^{(-)} | T | i) / (M_j^{(-)} | T | i)$ . If the tilde representation is considered, the relations  $\Re(\tilde{\kappa}^{cc}) = 0$  and  $\tan \tilde{\beta} \tan \delta_r = -\tilde{\xi}^2$  holding for it may be used to put Eq. (14) into a Beutler-Fano form:

$$|\tilde{\mathbf{D}}_j^{(-)}|^2 = |(\tilde{M}_j^{(-)} | T | i)|^2 \frac{|-\cot \delta_r + \tilde{q}_j|^2}{\cot^2 \delta_r + 1}. \quad (15)$$

$|\tilde{\mathbf{D}}_j^{(-)}|$  equals  $|\mathbf{D}_j^{(-)}|$  since  $\tilde{\Psi}_j^{(-)}$  differs from  $\Psi_j^{(-)}$  by  $\exp(i\pi\mu_j)$ [7, 14]. Phase renormalization does not change the absolute magnitude of a transition dipole matrix element but is instrumental in making the transition dipole matrix element into a Beutler-Fano form since the latter is only obtained in the tilde representation, or in the one obtainable from the tilde representation by the phase renormalization which keeps the eigenphase sum of physical scattering matrix unchanged.

For the resonance-centered representations, the physical incoming wavefunctions may be expressed as  $\Psi_j^{(-)} = e^{-i\delta_r} (M_j^{(-)} \cos \delta_r + iN_j^{(-)} \sin \delta_r)$ , which shows that  $M_j^{(-)}$  is the sole contributor to the physical incoming-waves at the energy where the phase shift  $\delta_r$  due to the resonance is zero. Its comparison with CM’s physical incoming wavefunction[25]

$$\Psi_E^{-(j)}(\text{CM}) = e^{-i\delta_r} \left\{ \psi_E^{-(j)} \cos \delta_r + i \left[ \left( 1 - |\psi_E^{(a)}\rangle \langle \psi_E^{(a)}| + \frac{i\Phi}{\pi(\sum_k |V_{kE}|^2)^{1/2}} \langle \psi_E^{(a)}| \right) \psi_E^{-(j)} \right] \sin \delta_r \right\} \quad (16)$$

suggests a one-to-one correspondence between  $M_j^{(-)}$  and  $\psi_E^{-(j)}$  and also between  $N_j^{(-)}$  and the term inside the square brackets which constitutes the second term inside the curly braces of the right-hand side of Eq. (16). The one-to-one correspondence between  $M_j^{(-)}$  and  $\psi_E^{-(j)}$  can also be seen in the asymptotic forms: the open channel part of the decoupled form  $\sum_{i \in P} \Phi_i(\phi_i^+ \delta_{ij} - \phi_i^- \sigma_{ij}^{oo}) - \Phi_c(\phi_c^+ + \phi_c^-)[(1 + S^{cc})^{-1} S^{co}]_{cj}$  of  $M_j^{(-)}$  ( $R \geq R_0$ ) is identical to the asymptotic form of  $\psi_E^{-(j)}$  if the one-to-one correspondence between  $\sigma^{oo}$  and  $\mathbf{S}_B$  is taken into account. The decoupled form, however, contains an additional closed channel term which rises exponentially at large  $R$ , showing that  $M_j^{(-)}$  by itself is not a physically acceptable wavefunction in contrast to the background one. But its contribution to cross-sections is still finite since it is multiplied by an initial wavefunction that may be reasonably assumed to be bound. This indicates that the background part  $\mathbf{S}_B$  of the scattering matrix  $\mathbf{S}$  ( $=\mathbf{S}_B \mathbf{S}_R$ ) of CM actually contains closed channel contributions. The closed channel contribution into  $M_j^{(-)}$  is given by the form of  $\phi_c^+ + \phi_c^-$  which is equal to  $i$  times the irregular function  $g_i$ . It shows that the regular function for the closed channel contributes nothing to  $M_j^{(-)}$ , presumably indicating that  $M_j^{(-)}$  is the form of minimal closed channel contribution in the intermediate and reaction zones and thus in the observables. This claim requires further study for sure.

Eq. (15) may be used to obtain  $|\langle \tilde{M}_j^{(-)} | T | i \rangle|^2$ ,  $\Re(\tilde{q}_j)$ ,  $\Im(\tilde{q}_j)$ ,  $\mu_c$ , and  $\tilde{\xi}^2$  from the experimental data using the method developed in the field of modeling of data[26] (the form of  $\beta$  as a function of energy needed for data fitting is given analytically for most fields but should be obtained numerically for the zero field using the Milne procedure described in Ref. [22]). But Eq. (15) is not expressed in terms of parameters whose physical origins are clearly identified. The r-representation may be used for that purpose since the channel coupling strength can only be completely disentangled there from the geometrical factors and the formulation is additionally simplified too by the fact that only one open process can be involved there for the resonance. Introducing the r-representation is equivalent to visualizing the photofragmentation process as being excited to eigenchannels of  $\mathbf{S}_r$  but observed in the detector through their projections to the detector eigenchannels. By the fact that  $\mathbf{S}_r$  is already diagonalized as  $\exp(-2i\delta_r \mathbf{p}_r)$  with eigenvalues  $\{\exp(-2i\delta_r), 1, \dots, 1\}$  and  $K_r^{cc} = 0$ , the well-known formulas for the eigenchannel wavefunctions  $\Psi_{r_k}^{(\text{eig})}$  given as the superpositions of

standing-waves[14], i.e.  $\Psi_{r_k} \cos \delta_k + \Psi_{r_c} Z_{rck} \cos \tilde{\beta}_c$  with  $Z_{rck} \cos \tilde{\beta}_c = -(\tan \tilde{\beta}_c)^{-1} (K_r^{co} \cos \delta)_{ck}$ , become reduced to  $\Psi_{r1} \cos \delta_r + \Psi_{r_c} \sin \delta_r / \tilde{\xi}$  for  $k = 1$  and  $\Psi_{r_k}$  otherwise. The transition dipole moments to  $\Psi_{r_i}^{(\text{eig})}$  can, then, be obtained as

$$\begin{aligned} \mathbf{D}_{r1}^{(\text{eig})} &= -(\Psi_{r1} | T | i) \frac{\tan \tilde{\beta} / \tilde{\xi}^2 + q_r}{(\tan^2 \tilde{\beta} / \tilde{\xi}^4 + 1)^{1/2}}, \\ \mathbf{D}_{r_k}^{(\text{eig})} &= (\Psi_{r_k} | T | i), \quad (k \neq 1) \end{aligned} \quad (17)$$

with the line profile index  $q_r$  defined as  $q_r = -(\Psi_{r_c} | T | i) / [\xi (\Psi_{r1} | T | i)]$ , which is clearly real because the standing waves  $\Psi_{r1}$  and  $\Psi_{r_c}$  are real[27]. From the unitary relation between  $\tilde{\mathbf{D}}_j^{(-)}$  and  $\mathbf{D}_{r_j}$ , we have  $\sum_{j \in P} |\tilde{\mathbf{D}}_j^{(-)}|^2 = \sum_{k \in P} |\mathbf{D}_{r_k}^{(\text{eig})}|^2$ . Using this relation, Eq. (15) becomes

$$\begin{aligned} \sum_{j \in P} |\tilde{\mathbf{D}}_j^{(-)}|^2 &= |(\Psi_{r1} | T | i)|^2 \frac{(\tan \tilde{\beta} / \tilde{\xi}^2 + q_r)^2}{\tan^2 \tilde{\beta} / \tilde{\xi}^4 + 1} \\ &\quad + \sum_{k \in P}' |(\Psi_{r_k} | T | i)|^2, \end{aligned} \quad (18)$$

where the prime on the summation symbol denotes that  $k = 1$  is excluded in the summation. Eq. (18) directly corresponds to the well-known total cross-section formula  $\sigma_{\text{tot}} = \sigma_a(\epsilon + q)^2 / (\epsilon^2 + 1) + \sigma_b$  of CM for photofragmentation in the neighborhood of an isolated resonance if the one-to-one correspondence between  $\Psi_{r1}$  and  $\psi_E^{(a)}$ , described below, is taken into account[16].

Since  $\tilde{\Psi}_j^{(-)}$  and  $\Psi_{r_k}^{(\text{eig})}$  are energy-normalized and related by a unitary transformation, their transition dipole moments are also related by the same unitary transformation as  $\tilde{\mathbf{D}}_j^{(-)} = \sum_{k \in P} \mathbf{D}_{r_k}^{(\text{eig})} (\tilde{\Psi}_j^{(-)} | \Psi_{r_k}^{(\text{eig})})$ . Using the transformation relation  $(\tilde{\Psi}_j^{(-)} | \Psi_{r1}^{(\text{eig})}) = \exp(i\delta_r) (\tilde{M}_j^{(-)} | \Psi_{r1})$  and  $(\tilde{\Psi}_j^{(-)} | \Psi_{r_k}^{(\text{eig})}) = (\tilde{M}_j^{(-)} | \Psi_{r_k})$  ( $k \neq 1$ ) derived in Appendix A and the formulas for  $\mathbf{D}_{r_k}^{(\text{eig})}$  given in Eq. (17), the transition dipole moment to the  $j$ -th fragmentation channel can be obtained as

$$\begin{aligned} \tilde{\mathbf{D}}_j^{(-)} &= (\tilde{M}_j^{(-)} | T | i) \left[ \frac{\tan \tilde{\beta} / \tilde{\xi}^2 + q_r}{\tan \tilde{\beta} / \tilde{\xi}^2 + i} \frac{(\tilde{M}_j^{(-)} | \Psi_{r1}) (\Psi_{r1} | T | i)}{(\tilde{M}_j^{(-)} | T | i)} \right. \\ &\quad \left. + \sum_{k \in P}' \frac{(\tilde{M}_j^{(-)} | \Psi_{r_k}) (\Psi_{r_k} | T | i)}{(\tilde{M}_j^{(-)} | T | i)} \right]. \end{aligned} \quad (19)$$

Let us define  $\tilde{\rho}_j$  as

$$\tilde{\rho}_j = \frac{(\tilde{M}_j^{(-)} | \Psi_{r1}) (\Psi_{r1} | T | i)}{(\tilde{M}_j^{(-)} | T | i)} = \frac{(P_{r1} \tilde{M}_j^{(-)} | T | i)}{(\tilde{M}_j^{(-)} | T | i)} \quad (20)$$

with  $P_{r1} = |\Psi_{r1}\rangle\langle\Psi_{r1}|$  in analogous to  $\rho_j$  of CM (identical to Starace's  $\alpha^*(jE)$  [17]) defined as  $(P_a\psi_E^{-(j)}|T|i)/(\psi_E^{-(j)}|T|i)$  with  $P_a = |\psi_E^{(a)}\rangle\langle\psi_E^{(a)}|$  [18]. (Notice that all the representations connected by the phase renormalization have the common value of  $\tilde{\rho}_j$ . This is consistent with the fact that phase renormalization does not change the absolute magnitude of a transition dipole matrix element.) Then it may be shown that the second term inside the brackets of the right-hand side of Eq. (19) is just  $1 - \tilde{\rho}_j$ . Substituting this and Eqs. (20) into Eq. (19), we obtain Eq. (15) but now with  $\tilde{q}_j$  expressed in terms of parameters  $q_r$  and  $\tilde{\rho}_j$  of clear physical origin as

$$\tilde{q}_j = q_r \tilde{\rho}_j + i(1 - \tilde{\rho}_j). \quad (21)$$

Before, we claimed that not  $\tilde{\Psi}_j^{(-)}$  but  $\tilde{M}_j^{(-)}$  corresponds to the background wavefunction  $\psi_E^{-(j)}$  of CM. A similar correspondence may be claimed for  $M_{ri}^{(-)}$ . But, for the r-representation,  $M_{ri}^{(-)}$  equals  $\Psi_{ri}$ , as shown in Appendix A. Therefore, we claim that  $\Psi_{ri}$  corresponds to CM's  $\psi_E^{(a)}$  for  $i=1$  and  $\psi_E^{(\lambda)}$  ( $\lambda \neq a$ ) otherwise. Notice that  $\Psi_{ri}$  are real quantities as are  $\psi_E^{(\lambda)}$ , which is the reason why  $\Psi_{ri}$  is used preferably to  $M_{ri}^{(-)}$  in the above equations. The claim is bolstered by the same one-to-one correspondence between wavefunctions found from the comparison of MQDT's  $\tilde{\rho}_j$  with CM's  $\rho_j$ . Here, we only talked about the analogy between formulas of two theories not the actual relations of corresponding terms in two theories. The relations may be derivable from the prescription described in Ref. [14]. For example, it may be found that  $\Psi_{ri}$  equals  $\psi_E^{(a)} + i\tilde{\xi}\Phi_c(\phi_c^+ + \phi_c^-) + O(\tilde{\xi}^2)$  for  $i = 1$  and  $\psi_E^{(\lambda)} + O(\tilde{\xi}^2)$  ( $\lambda \neq a$ ) otherwise.

Finally, let us consider about dynamical parameters extractable from the total and partial photofragmentation cross-sections. Since total cross-sections are proportional to  $\sum_{j \in P} |\tilde{D}_j^{(-)}|^2$ , Eq. (18) may be used to fit the experimental data of total cross-sections. Levenberg-Marquardt method [26] may be employed for such a data fitting to obtain the information on  $|\langle\Psi_{r1}|T|i\rangle|^2$ ,  $\sum_{j \in P'} |\langle\Psi_{rj}|T|i\rangle|^2$ ,  $q_r$ ,  $\tilde{\xi}^2$ , and  $\mu_c$ . Information on the absolute value of  $\langle\Psi_{rc}|T|i\rangle$  and its relative sign to  $\tilde{\xi}\langle\Psi_{r1}|T|i\rangle$  may be obtained from  $q_r$ , since it is defined as  $-(\Psi_{rc}|T|i)/[\tilde{\xi}(\Psi_{r1}|T|i)]$ . For the partial cross-sections,  $|\tan\tilde{\beta}/\tilde{\xi}^2 + \tilde{q}_j|^2/(\tan^2\tilde{\beta}/\tilde{\xi}^4 + 1)$  is changed to the form consisted of real terms as  $[\tan\tilde{\beta}/\tilde{\xi}^2 + \Re(q_j)]^2/(\tan^2\tilde{\beta}/\tilde{\xi}^4 + 1) + [\Im(q_j)]^2/(\tan^2\tilde{\beta}/\tilde{\xi}^4 + 1)$ , which may be used to extract  $\Re(\tilde{q}_j)$  and  $[\Im(\tilde{q}_j)]^2$ . Notice that the data fitting leaves the sign of  $\Im(\tilde{q}_j)$  undetermined. After  $\tilde{q}_j$  is obtained up to the sign of its imaginary part,  $\tilde{\rho}_j$  is obtainable from the relation  $\tilde{q}_j = q_r \tilde{\rho}_j + i(1 - \tilde{\rho}_j)$ , which yields the quadratic equation for  $\tilde{\rho}_j$  and eventually gives two  $\tilde{\rho}_j$  compatible with both  $\tilde{q}_j$  and  $\tilde{q}_j^*$ . From  $\tilde{\rho}_j$ , the information is obtained on the projection factor  $(\tilde{M}_j^{(-)}|\Psi_{r1})$

since other factors like  $(\Psi_{r1}|T|i)$  and the absolute magnitude of  $(\tilde{M}_j^{(-)}|T|i)$  constituting  $\tilde{\rho}_j$  are already obtained. The projection factor is related to the component of  $\tilde{\xi}$  but not directly because the latter pertains to the eigenchannels of  $\tilde{\sigma}^{oo}$ . The relation is given by  $|\tilde{\xi}_k/\tilde{\xi}| = |\sum_{j \in P} \tilde{U}_{kj}^T(\tilde{M}_j^{(-)}|\Psi_{r1})|$  where absolute value is taken to get rid of an unimportant phase factor.

#### IV. SUMMARY AND DISCUSSION

We confirmed again, for the case involving one closed and many open channels, the striking similarities between MQDT and CM formulas found for the case involving one closed and two open channels [14] if MQDT is reformulated by means of Giusti-Suzor and Fano's phase renormalization and Lecomte and Ueda's additional orthogonal transformation. The unitarity of  $\tilde{\sigma}^{oo}$  [ $\equiv (1 - i\tilde{K}^{oo})(1 + i\tilde{K}^{oo})^{-1}$ ] and its simultaneous diagonalizability with  $\tilde{K}^{oo}$  by the same orthogonal transformation are newly found to play the pivotal role in the reformulation. By this reformulation, we found the one-to-one correspondence between two different manifestations,  $\tilde{M}_j^{(-)}$  and  $\Psi_{rj}$ , of the form  $\Psi_j^{(-)} + \Psi_c^{(-)}[K^{co}(-i + K^{oo})^{-1}]_{cj}$  of MQDT and the background wavefunction  $\psi_E^{-(j)}$  and Fano's 'abc.' states of CM, respectively, and also between  $\tilde{\sigma}^{oo}$  of MQDT and the background scattering matrix  $\mathbf{S}_B$  of CM. Under this correspondence, formulas in both theories exactly coincide with each other when further one-to-one correspondence coming from the extension of  $-\cot\delta_r = 2(E - E_0)/\Gamma$  of CM to  $\tan\delta_r \tan\tilde{\beta} = -\tilde{\xi}^2$  of MQDT taken into account. Note that the reformulation allows MQDT to have the full power of the CM theory, still keeping its own strengths such as the fundamental description of resonance phenomenon without any assumption of the presence of a discrete state as in CM.

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#### APPENDIX A: TRANSFORMATION RELATIONS AMONG VARIOUS WAVEFUNCTIONS

Here, we want to prove the relations  $(\tilde{\Psi}_j^{(-)}|\Psi_{r1}^{(\text{eig})}) = \exp(i\delta_r)(\tilde{M}_j^{(-)}|\Psi_{r1})$  and  $(\tilde{\Psi}_j^{(-)}|\Psi_{ri}^{(\text{eig})}) = (\tilde{M}_j^{(-)}|\Psi_{ri})$  ( $i \neq 1$ ), which can be recast as  $(\tilde{\Psi}_j^{(-)}|\Psi_{ri}^{(-)}) = (\tilde{M}_j^{(-)}|\Psi_{ri})$  by means of the relation between eigenchannels and incoming-waves in the r-representation given

by  $\Psi_{r_i}^{(\text{eig})} = \Psi_{r_i}^{(-)} \exp(i\delta_r)$  for  $i = 1$  and equals otherwise. Let us consider the transformation from the tilde representation into the r-one. It is performed by two transformations  $T(0, \tilde{\delta}^0, \tilde{U})$  and  $T(0, 0, U_r)$ . If we denote the  $N_0 \times N_0$  unitary transformation  $\tilde{U} \exp(i\tilde{\delta}^0) U_r$  as  $V$ , then, from the definition of the transformation extended by Lecomte and Ueda, the following transformation relations are obtained:  $\Phi_j \phi_{r_j}^+ = \sum_{i \in P} \Phi_i \tilde{\phi}_i^+ V_{ij}$  and  $\Phi_j \phi_{r_j}^- = \sum_{i \in P} \Phi_i \tilde{\phi}_i^- V_{ij}^*$  for  $j \in P$  and  $\Phi_c \phi_{r_c}^\pm = \Phi_c \tilde{\phi}_c^\pm$  for  $j \in Q$ . Substituting into the decoupled form of  $\Psi_{r_i}^{(-)}$  in  $R \geq R_0$  and after rearrangement, we obtain  $\Psi_{r_i}^{(-)} = \sum_{j \in P} \tilde{\Psi}_j^{(-)} V_{ji}$  ( $i \in P$ ). Likewise, we obtain  $\Psi_{r_i}^{(-)} = \sum_{j \in P} \tilde{\Psi}_j^{(-)} V_{ji}$ .  $V_{ji}$  may be denoted in Dirac notation as either  $(\tilde{\Psi}_j^{(-)} | \Psi_{r_i}^{(-)})$  or  $(\tilde{\Psi}_j^{(-)} | \Psi_{r_i}^{(-)})$ , with the precaution that it should not be interpreted as an integral. Then showing that  $(\tilde{\Psi}_j^{(-)} | \Psi_{r_i}^{(-)}) = (\tilde{M}_j^{(-)} | \Psi_{r_i})$  is equivalent to showing that  $\Psi_{r_i} = \sum_{j \in P} \tilde{M}_j^{(-)} V_{ji}$  where  $i \in P$ . The proof hinges on the following relation:

$$\tilde{M}_j^{(-)} = \tilde{\Psi}_j^{(-)} + i\tilde{\xi} \tilde{\Psi}_c^{(-)} V_{1j}^\dagger. \quad (\text{A1})$$

Let us derive the relation. The coefficient of  $\tilde{\Psi}_c^{(-)}$  of

Eq. (13), i.e.,  $[\tilde{K}^{co}(-i + \tilde{K}^{oo})^{-1}]_{ck}$ , can be recast as  $-(\tilde{S}^{cc} + 1)^{-1} \tilde{S}^{co}$ . From  $\tilde{S}^{cc} = S_r^{cc}$ ,  $\tilde{S}^{co} = S_r^{co} V^\dagger$  and  $(S_r^{cc} + 1)^{-1} S_r^{co} = -i\tilde{\xi}(1, 0, \dots, 0)$ , Eq. (A1) is easily obtained. Now, from the relation  $\Psi_{r_i} = \sum_{j \in P, Q} \Psi_{r_j}^{(-)} (1 + iK_r)_{ji}$  between the standing-waves and incoming-waves with  $i \in P$  hereinafter, one obtains

$$\Psi_{r_i} = \Psi_{r_i}^{(-)} + i\tilde{\xi} \Psi_{r_c}^{(-)} \delta_{1i}. \quad (\text{A2})$$

Substituting Eq. (A1) into  $\Psi_{r_i}^{(-)} = \sum_{j \in P} \tilde{\Psi}_j^{(-)} V_{ji}$ ,  $\Psi_{r_i}^{(-)}$  can be expressed as  $\sum_{j \in P} \tilde{M}_j^{(-)} V_{ji} - i\tilde{\xi} \tilde{\Psi}_c^{(-)} \delta_{1i}$ , from which one finally obtains  $\Psi_{r_i} = \sum_{j \in P} \tilde{M}_j^{(-)} V_{ji}$ . Comparison of this with  $\Psi_{r_i}^{(-)} = \sum_{j \in P} \tilde{\Psi}_j^{(-)} V_{ji}$  proves that  $(\tilde{\Psi}_j^{(-)} | \Psi_{r_i}^{(-)})$  equals  $(\tilde{M}_j^{(-)} | \Psi_{r_i})$ . Notice that the right-hand side of Eq. (A2) is equal to  $M_{r_i}^{(-)}$  so that  $\Psi_{r_i} = M_{r_i}^{(-)}$ . Since the projection factor  $(\tilde{M}_j^{(-)} | \Psi_{r_i})$  corresponds to  $(\psi_E^{(-j)} | \psi_E^{(a)})$  of CM, the equality  $(\tilde{M}_j^{(-)} | \Psi_{r_i}) = (\tilde{M}_j^{(-)} | M_{r_i}^{(-)})$  emphasizes that  $M^{(-)}$  functions correspond to the background wavefunction shorn of the configuration mixing with a discrete state.

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